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Bozok Science Workshop 2017, Yozgat, August 23-25, 2017.

Preface to the Special Issue for BSW2017

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This special issue of Electronic Letters on Science & Engineering (e-LSE), An International open access Journal, includes the abstracts of the presentations at the workshop, BSW2017 (Sixth Bozok Science Workshop: Studies from Nuclei to Nanomaterials with Applications) held during August 23-25, 2017 at Bozok University, Yozgat, Turkey.

At the workshop the discussions were based on active researches from basic to several applied fields. The fundamental scientific philosophy behind the traditional meeting, Bozok Science Workshops, is the stimulation of cross-disciplinary flow of knowledge and expertise from both the experimental and theoretical standpoints. At the first, second, third, fourth and fifth workshops the main topics were chosen as "Boron studies in nano-scale" for BSW2010, "Computational Chemical Physics" for BSW2011, "Computational Studies on Structure and Dynamics from Nuclei to Biological Molecules" for BSW2012, "Studies on Structure and Dynamics from Nuclei to Clusters" for BSW2013 and "Nano carbon materials and their applications" for BSW2016, respectively. Despite of the considered special topics, the studies on boron, computational chemical physics, any nanomaterilas, atomic/molecular and cluster systems were still welcome again to BSW2017.

As for the workshop planned to be held as BSW2017; the abstracts are prepared as a special issue of e-LSE. All referees (consisting 38 experts and 7 of them from out of Turkey) have been selected from the Scientific Committee (consisting 54 experts and 10 of them from out of Turkey) of BSW2017 to review the abstracts before the workshop. In order to take part at the above mentioned special issue; presenting the selected abstract by applicant is the main principle.

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By means of the workshop and this special issue of e-LSE, we hope to give opportunity to the authors to improve the quality of their works also give the same opportunity to the referees to make critics and to be aware of the active studies submitted to the meeting. Announcement on the special issue is on the workshop circulars right from the start, at web page and in the shared emails. In total, 36 selected abstracts from the reviewed and presented abstracts are published in this issue. This e-LSE issue may be a good reference material and be a great source for the experts who are interested in the discussed topics.

I am pleased to be Editor of this special issue of e-LSE. I would like to thank to the Scientific Committee for the generous support for recommending invited lectures, subjects and sharing their opinion to improve the workshop. Especially, I would like to thank to the members accepting my invitations to be referee for selecting the abstracts for this volume, and to the members of the Organizing Committee for their help. Finally, I would like to thank to Founding Editor Dr. Feyzullah Temurtaş for giving me this opportunity and helping me in managing this issue.

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The Synthesis and Characterization of New Boron and its Derivatives and Their Anticancer, Antimicrobial and Antioxidant Activities

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Abstract: The chemistry of elemental boron, its compounds and crystalline phases based on them is currently a vast and quite complicated scientific field at the boundary of inorganic and organo-element chemistry. Boron and its derivatives are used in areas from agriculture to industry, such as glass, ceramic, textile, automotive, electronics and nuclear industry, medicine, pharmaceutical and cosmetic industry, energy, construction industry, and communication tools and detergent. Due to the widespread use of boron compounds, the synthesis and application of these systems in science and technology have attracted attention. Boronic acid compounds with different substituted groups were handled to synthesize various ligands encoded as B1, B2, B3, B4, B5, B6, B7 and B8. B5 and B7 were tested for the cytotoxic activity against the prostate cancer cells and it was found that the cell viability of cancer cells was decreased while most of the healthy cells could still be viable. 5 mu M solutions of B5 and B7 decreased the cell viability to 33% and 44% whereas healthy cells were 71% and 95%, respectively, after treatment. Antimicrobial properties were explored against the bacterial and fungal microorganisms with B1, B5 and B7. The inhibition zones were evaluated for all boronic structures, and the growth inhibition zones were determined in a range of 713 mm diameter for different microorganism species. Staphylococcus aureus was the common microorganism that three boronic compounds with imine ligands showed the activity. Antioxidant features of B2, B3, B4, B5, B6, B7 and B8 were investigated by different processes such as Beta-carotene bleaching (BCB), 2,2-diphenyl picryl hydrazyl (DPPH), 2,2'-azino-bis(3-ethylbenzothiazoline-6-sulphonic acid) (ABTS) and Cupric reducing antioxidant capacity (CUPRAC) methods. Significant antioxidant activity was achieved by the phenyl boronic based ligands and these compounds demonstrated as much activity as standards (alpha-Toc and BHT).

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Keywords: *Boron, anticancer, antioxidant, antimicrobial*

References:

[1] Paşa, S., *et. al.*, Journal of Pharmaceutical Analysis 6 (2016) 39–48.

[2] İlhan, S., PhD Thesis, Çeşitli Makrosiklik Schiff Bazlarının ve Template Etki ile Komplekslerinin Sentezi ve Karakterizasyonu, Dicle University, Institute of Science, 2006.

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Thermal and Dielectric Properties of Polypyrrole-Clay Composites

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Abstract: In this study, polypyrrole-clay (PPy-Clay) composites were prepared by the in situ chemical oxidative polymerisation of pyrrole in the presence of clay. The chemical structures of the composites were characterised by FTIR and XRD analysis. The thermal properties of these novel composites were analysed by TGA and DSC measurements. Glass-transition temperatures and char yields increased with the increase of clay content in the nanocomposites. The interactions between PPy and clay were mainly between polypyrrole and the layers of clay. It was observed that, as the amount of clay in the composites increased, the dielectric permittivity decreased while the dielectric conductivity of the composite materials increased.

Keywords: *Composite, polypyrrole, clay, dielectric*

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Integrated Use of Municipal Solid Waste And Industrial Waste as Renewable Energy Source

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Abstract: Rapidly developing industrialization, urbanization; due to the technological innovations, rising standard of living by the development of modern medicine and the population increase related to it have increased consumption of energy and raw materials in every area. One of the serious consequences of this development is the environmental pollution problem.

One of the sustainable energy sources that do not lead to environmental pollution is biomass energy. Biomass is the general name of all unfossilized biomass obtained from living or recently lived creatures. Biomass is an energy source and can be used either as a fuel for biological substances or for industrial purposes [1]. The three main sources of biomass energy, industrial and municipal wastes, agricultural-livestock wastes and forest-based wastes are used as raw materials [2].

End-of-life tire is defined as a tire is considered at the end of its life when it can no longer be used on vehicles (after having been retreaded or regrooved) [3]. The sources as industrial wastes and the byproducts resulting from the processing of municipal solid wastes and ELTs are frequently used as biomass sources. In general, Direct Burning, Gasification and Pyrolysis technologies are used for recycling and recovery of these wastes.

In this study, two incineration plants in Germany and a biogas plant in Afyon were introduced. In addition, the theoretical study results were presented for a plant scenario of 3.5 MW power fed with municipal solid waste and ELTs.

The aim of the dissemination and promotion of facilities related to the use of renewable energy resources in our country is among the primary objectives of our university. In this context, infrastructure works have been accelerated and many facilities in different countries have been

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studied technically. The impressions obtained at the end of these examinations have been shared with interested parties within the scope of this study.

Keywords: Renewable energy source, Pyrolysis technology, Biomass energy.

References:

[1] Brown. S., (1997), Estimating Biomass and Biomass Change of Tropical Forests: A Primer, Forest Resources Assessment publication

[2] http://www.environbusiness.com/eeae/biomass

[3] Full report of World Business Council for Sustainable Development, WBCSD, November 2008, ISBN:978-3-940388-31-5

Electronic Letters on Science & Engineering 13 (2) (2017)
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Comparison of n-CB Liquid Crystals by Light Scattering

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Abstract: The computer modelling of light scattering and its propagation through n-CB (n-cyanobiphenyl) liquid crystals, shaped slab has been compared. Light propagation through a slab has been represented via transmitted and reflected electromagnetic fields by using a finite thin layers model. Numerical aspects of the light scattering process, which are based on numerically solving Maxwell's equations, have been calculated for n-CB liquid crystals. It has been described in detail computation the circular slab model for computing light scattering from a layered liquid crystals and the results of benchmark computations have been presented for the considered model. These results are associated with our previous studies [1-4] on different geometries by light scattering.

Keywords: *Light scattering; n-CB liquid crystals; slab; computer modelling*

References:

[1] Yılmaz, S., Journal of Modern Optics, 59 (2012) 912-916.

[2] Yılmaz, S., Journal of Quantative Spectroscopy & Radiative Transfer, 104 (2007) 305-309.

[3] Yılmaz, S., Kalkandelen, A., Isayeva, N., Journal of Quantative Spectroscopy & Radiative Transfer, 97 (2006) 20-28.

[4] Yılmaz, S., Koç, H., Molecular Physics, 103 (2005) 2633-2537.

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Atomic Structure of Graphene Supported Hollow Ag Cubic Nanoparticles Under CO Gas Adsorption by Molecular Dynamics Simulations

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Abstract: The metallic nanoparticles on graphene sheets as namely metallic/graphene nanocomposites are a new generation of materials with promising applications such as energy and storage systems, catalysts and chemical and bio-sensors. In this contribution, we can add specific properties of this new class of graphene based nano composites uses noble metals to the already mentioned characteristics of graphene. The effect of size and hollow cavity on Ag cubic nanoparticles (NPs) supported by graphene in vacuum and CO gas have studied by molecular dynamics (MD) simulations. The reversibility of atomic structure for those NPs has discussed.

Here, we have considered two different sizes of hollow Ag cubic NPs with two layers of graphite sheets contained 8400 carbon atoms. First, the atomic structure based properties of the free standing hollow Ag nanoparticles have obtained at different temperatures under heating. Then we have fixed the graphene, and hollow metallic cubic Ag NPs/graphene nano-composite system has placed with graphite sheets in a vacuum, and randomly distributing the CO gas, respectively. The atomic structure analysis for the NPs/ nanocomposite system has computed by the common neighbour analysis (CNA), bond angle analysis (BAA), radial distribution functions and atomic self diffusion coefficients of particles.

We have found that because of the surface atoms, the small size of the graphene supported hollow Ag cubic NPs have more stable structure than that of the bigger size of NPs contrast with similar size of the free standing ones. Thus temperature dependency is more significant for small NPs. The results agree well with those obtained for solid Ag/graphene nanocomposites. It has demonstrated that the CO gas/graphene composite condition changes the atomic structure and diffussivity of the hollow

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NPs more significantly than that of the NPs in a vacuum. In addition to that, the reversibility of structural changes is important for sensor applications. The selection of appropriate size and cavity diameter of hollow NPs to use them in gas sensor applications need to more experimental and theoretical investigations.

Keywords: *Hollow Ag nanoparticles, graphene, CO gas adsorption*

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The Investigation of Structural and Dynamical Properties of Au-Pd Nanoalloys Supported on MgO(001) Surface

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Abstract: Bimetallic nanoparticles composed of Au and Pd transition metals have been shown high catalytic performance in various reactions such as hydrogenation and oxidation. Metal oxide surfaces have been enhanced the catalytic performance of the nanoalloys. Due to the oxide surface, significant changes in electronic and magnetic properties as well as catalytic properties caused the investigation of the nanoalloys depending on size. In the present study, the structural and dynamical properties of both pure and bimetallic nanoalloys composed of Au and Pd transition metals supported on MgO (001) surface were investigated as having ratios of Au_nPd_n (%50-%50), Au_nPd_{3n} (%25-%75) and $Au_{3n}Pd_n$ (%75-%25) in terms of atomic number. The global minimum structures of Au-Pd nanoalloys have been obtained by Basin-Hopping algorithm. To describe the interatomic interactions, the Gupta many body potential energy function was used. Then the melting behavior of Au-Pd nanoalloys on MgO (001) surface were investigated by canonical molecular dynamics simulation method. As a results of the global optimization, some of the pure Au and Pd clusters were deposited by (001) epitaxy on MgO(001) surface and some clusters were deposited (111) epitaxy on surface. Unlike pure metal clusters, Au-Pd bimetallic nanoalloys tend to settle with (001) epitaxy in accordance with the oxide surface.

Keywords: *Nanoalloys, MgO surface, Optimization*

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Synthesis and Antioxidant Activities of New1-Acetyl-3-Alkyl(Aryl)-4-[3-Ethoxy-2-(p-Methoxybenzoxy)-Benzylidenamino]-4,5-Dihydro-1H-1,2,4-Triazol-5-One

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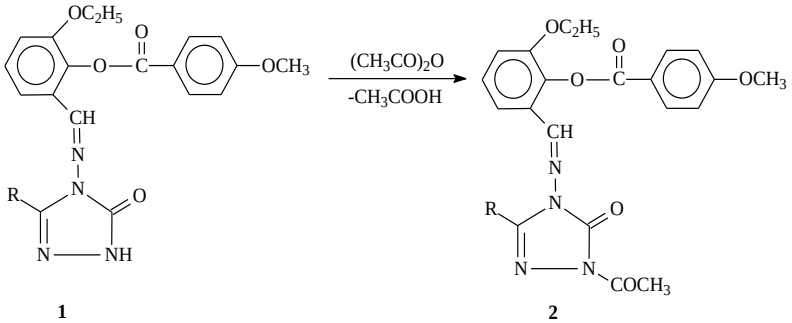
Abstract: 1,2,4-Triazole derivatives have drawn considerable attention for the past few decades because of their diverse biological properties. Many 1,2,4-triazole derivatives are found to be potent antioxidant, anti-inflammatory, antimicrobial and antiviral agents. The identification of triazoles and determination of their antibacterial activities are of considerable interest because of the role they play in pharmacological actions [1-4]. In this study, firstly five novel 1-acetyl-3-alkyl(aryl)-4-[3-ethoxy-2-(p-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1H-1,2,4-triazol-5-ones (2) were synthesized by the reactions of 3-alkyl(aryl)-4-[3-ethoxy-2-(p-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1H-1,2,4-triazol-5-ones (1) [5] with acetic anhydride. In order to identify new compounds synthesized in the study, spectroscopic methods including IR, ^{1}H-NMR, ^{13}C-NMR and UV were used. In the second part of the study, antioxidant activities of the newly synthesized compounds were screened using different antioxidant methodologies: free radical scavenging activity [5], reducing power activity [7] and metal chelating activity [8].



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Acknowledgements: This work was supported by the Scientific Research Projects Coordination Unit of Kafkas University (Project Number: 2011-FEF-31).

Keywords: *Triazole, Antioxidant, Alkil/Aril, Methoxybenzoxy*

References:

[1] Henen, MA., *et. al.*, Med. Chem. Res., 21 (2012) 2368-2378.

[2] Kahveci, B., *et. al*., Russ. J. Org. Chem., 44 (2008) 1816-1820.

[3] Unver, Y., *et. al*., Turk J. Chem., 33 (2009) 135-147.

[4] Yüksek, H., *et. al*., Archiv der Pharmazie, 346 (2013) 470-480.

[5] Kardaş, F., *et. al*., 1. International Turkic Conference on Chemical Sciences and Technologies, Bosna-Herzegovina, (2015) P0-63.

[6] Blois M.S., Nature, 181 (1958) 1199-1200.

[7] Oyaizu M., Japanese J. Nutrition and Dietetics, 44 (1986) 307-316.

[8] Dinis TCP., Madeira VMC. & Almeida L.M., Archives of Biochem. and Biophysics, 315 (1994) 161-169.

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A Many - Body Model Suggestion for Deuterons and Electrons in an Inertial Electrostatic Confinement Fusion Device

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Abstract: Motivation on fusion energy explorations focuses on the experimental facilities related to TOKAMAKs, plasma focus machines, stellerators and inertial electrostatic confinement devices (IECD) and their theoretical interpretations due to the determination of their characteristic features and design problems. In such machines, the modeling of the plasma environment under a specific pressure and electromagnetic excitement becomes important since they influence on the production of fusion yields. In that context, the determination of scaling factor, plasma density and confinement time play important role.

According to our earlier studies [1,2], dynamics of particles in a fully - ionized media of IECD, there exist complicated motions including chaotic and regular ones. The proposed model includes equivalent numbers of electrons and ions inside the cell. Electrons and ions can intervene with each other and all interact with the device cathode, wall and the electromagnetic forces exerted by the electrical and magnetic potentials.

The simulations have been performed in MatLab package. Position, velocity, ion/electron temperatures, kinetic energy, ion density and particle distributions can be calculated from real – time simulations. Besides, the trajectories of each particle can be observed in three dimensions. The ion temperature increases by time substantially as the number of particles increase. In addition, the initial conditions of particles play important roles to confine them in the central grid.

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Keywords: *Radiation, inertial electrostatic confinement, fusion, Deuterium*

References:

[1] Dursun, B., Kurt, E., Kurt, H., Int. J. Hydrogen Energy, 42 (2017) 17874 – 17885.

[2] Dursun, B., Kurt, E., Int. J. Hydrogen Energy, 41 (2016) 12546-12554.

Electronic Letters on Science & Engineering 13 (2) (2017)
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The Deformation Effect on the Cross Section Calculations

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Abstract: We have currently studied on the effect of the deformation parameter of the target nucleus for the various reactions. We first investigated the nuclear structure of the target nuclei within the interacting boson model-1 (IBM-1). The parameters of the model Hamiltonian were fitted from the experimental data obtained at National Nuclear Data Center (NNDC) for the calculation of the energy levels of the target nuclei. Later these parameters were used in the formalism of the potential energy surface (PES) of IBM-1 to predict the geometric shape of the given targets and to determine the deformation parameter (β). To understand the effect of the β parameter, this parameter was used as an input in the TALYS 1.8 code for calculation of the cross sections of different projectiles. One of the recent applications, the deformation parameter obtained by IBM-1 for the target ^{110}Pd nucleus shows the positive effect on the cross section calculation for ^{110}Pd(d,n)^{111}Ag and ^{110}Pd(d,2n)^{110m}Ag reactions [1]. The different projectiles have been selected for the detail analyzing on other reaction types.

Keywords: *deformation parameter, interacting boson model, cross sections, TALYS code.*

References:

[1] M. Böyükata, İ. H. Sarpün, A. Aydın, Phys. Atom. Nucl. (accepted)

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Investigation of Temperature Dependent Current Transport Mechanism of Au/Al_2O_3/ n-Si Schottky Diode

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Abstract: This study, the forward bias current-voltage-temperature (I-V-T) characteristics of Au/ Al_2O_3/ n-Si Schottky diode were studied in the temperature range of 260-360 K. Al_2O_3 was deposited on n-Si substrate by atomic layer deposition (ALD). The main electrical parameters such as barrier height (Φ_{Bo}), ideality factor (n) and reverse saturation current (I_o) have been calculated by applying thermionic emission theory (TE). Additionally, series resistance (R_s) and Φ_{Bo} were calculated from the forward bias I-V data using the methods Norde. Experimental results show that I-V-T characteristics of the Au/ Al_2O_3/ n-Si Schottky diode can be explained on the basis of the TE theory with a double Gaussian distribution of the Schottky barrier heights.

Acknowledgements: This work is supported by The Management Unit of Scientific Research Project of Hitit University under Project Numbers FEF19002.15.001 and FEF19004.15.10.

Keywords: *Electrical properties; ALD; Au/n-Si/Al_2O_3 Schottky diode; Barrier Heights; Gaussian Distribution*

References:

[1] N. Hamdaoui, R. Ajjel , B. Salem , M. Gendry, Material. Sci. Semicon. Process. 26, 431 (2014)

[2] Ş. Altındal, H. Kanbur, İ. Yücedağ, A. Tataroğlu, Microelectron. Eng. 85, 1495 (2008)

[3] K. Ahmed, T. Chiang, Appl. Phys. Lett. 102, 042110 (2013)

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Electronic Letters on Science & Engineering 13 (2) (2017)
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Synthesis of Biocompatible and Eco-Friendly Graphene

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Abstract: Graphene is a hexagonal lattice structure of one atom thick layer that exhibits remarkable electronic, mechanic and thermal properties [1]. In the present study, graphene oxide (GO) was synthesized by the hummers method [2] and modified hummers method [3] and then GO was reduced by using reductant chemicals such as, hydrazine [4] and vitamin C [5]. Synthesized reduced graphene oxide (rGO) was characterized by transmission electron microscopy (CTEM), raman spectroscopy, elemental analysis and biocompatibility analysis.

The purpose was to compare the results that were obtained by different techniques. The chemically reduced graphene by vitamin C was examined by electron diffraction technique in the CTEM. The results showed that the structure consists of a mixture of single and few layers of rGO. The other outcome is that GO shows relatively good biocompatibility when the concentration is at 3,125 µg/mL and 6,25 µg/mL. Moreover, the excellent chemical reduction of GO with vitamin C does not contain toxic agents providing both the eco-friendly and the same high quality as other known techniques.

Acknowledgements: This work is supported by Kırıkkale University under grant number 2016/047.

Keywords: *Graphene, graphene oxide, rGO, Vitamin C, Biocompatibility*

References:

[1] A.K. Geim and K.S. Novoselov, Nature Materials, 6, 183, (2007).

[2] W.S. Hummers and R.E. Offeman, Journal American Chem. Soc., 80, 1339, (1958).

[*] *Corresponding author; Tel.: +(90) 506 6350953 E-mail: dilaraickecan@gmail.com*

[3] S. Liu S, *et. al*., ACS Nano 5, 6971, (2011).

[4] S. Stankovich, *et. al.*, Carbon 45, 1558, (2007).

[5] J. Gao, *et. al*., Chemistry of Materials, 22, 2213, (2010).

Electronic Letters on Science & Engineering 13 (2) (2017)
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The Comparison of Some Predictions of Davidson Like Potentials with Interacting Boson Model Results and X(5) Behaviors on $^{144-154}$Nd Isotopes

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Abstract: It has been carried out that the level scheme of the transitional nuclei $^{144-154}$Nd also presents the characteristic X(5) pattern, not only in the ground-state band but also in its some low-lying bands. An adequate point of the model leading to the X(5) symmetry is therefore confirmed. The positive parity states of even-mass Nd nuclei has also been carried out within the framework of interacting boson model and then the calculated energy values were compared with the experimental data along with the Davidson potential predictions. By comparing transitional behavior in the Nd nuclei with the predictions of an X(5) critical symmetry, an achievable degree of agreement was seen between the predictions of the model leading to this symmetry and the interacting boson models (IBM-1 and IBM-2). At the end, it was pointed out that they are nicely agree well with the predictions of the experimental data [1-5].

Keywords: *even even nuclei, Nd nuclei, Davidson potential, X(5) structure, interacting boson model*

References:

[1] J. Dalmasso, H. Forest, G. Ardisson, Phys. Rev. C 32, 1006-1009, (1985).

[2] T. Karlewski, *et. al.*,, Z. Phys. A 330, 55- 58, (1988).

[3] Y. Kawase, K. Okano, , Z. Phys.A 330, 231-234, (1988).

[4] J.B. Gupta, J. Phys. G 21, 565-575, (1995).

[5] J. Holden, *et. al.*, Phys. Rev. C 63, 024315, (2001).

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Study on the Electromagnetic Transition Probabilities for $^{78-86}$Sr Nuclei

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Abstract: Recently, we studied on some nuclear structural properties of $^{78-86}$Sr nuclei within the interacting boson model-1 (IBM-1). We investigated their band structure by calculating the energy levels, and the energy ratios. We compared the calculated energy levels with experimental data and completed the fitting procedure for Hamiltonian parameters. In this work, we have investigated the electromagnetic transition probabilities for $^{78-86}$Sr nuclei having the experimentally known B(E2) values. These B(E2) values were calculated by using computer code (PHINT) and compared with experimental data obtained at the National Nuclear Data Center (NNDC).

Keywords: *energy level, energy ratio, electromagnetic transition probabilities, B(E2) value, Sr nucleus, interacting boson model.*

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The Investigation of B(E2) Values in $^{82-88}$Zr Isotopes within IBM-1

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Abstract: In our recent study, we investigated the energy levels and energy ratios of $^{82-88}$Zr isotopes. Their energy levels in the ground-state (g.s.), gamma (γ) and beta (β) bands were calculated within the interacting boson model-1 (IBM-1) and compared with the experimental data. In this work, we have focused on the B(E2) values of $^{82-88}$Zr isotopes. The ^{82}Zr, ^{84}Zr nuclei have the E2 transitions in between the levels of the g.s. band and ^{86}Zr, ^{88}Zr nuclei have these transitions in between the levels of the g.s. and β bands. We calculated all experimentally known B(E2) values for $^{82-88}$Zr isotopes within the IBM-1 then compared with experimental data and they show generally good agreement.

Keywords: *B(E2) values, energy levels, interacting boson model, Zr isotopes.*

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Investigation of Ni-B Catalysts Obtained in Different Solutions in Hydrolysis of Sodium Borohydride

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Abstract: In this study, different catalysts were synthesized for hydrogen production from sodium borohydride solutions, which are considered as a hydrogen storage source in recent years, and the parameters related to hydrogen production were investigated by increasing the catalytic activities of these catalysts. In this study, the catalytic effects were increased by subjecting the catalysts to microwaves after synthesis, which was started to be used as a new method in recent years, and the effect of these catalysts on hydrogen production in the presence of sodium borohydride was investigated. In this study, Ni-based catalyst synthesis; After adding 1.5 g of $NiCl_2x6H_2O$ into 50 ml of ethanol, it is cooled to about 3-4 °C with stirring, then slowly adding 2.5% $NaBH_4$ solution. The resulted solution was then filtered and dried to obtain Ni-B catalyst. The obtained Ni-B catalyst was evaluated for its ability to produce hydrogen from sodium borohydride with increasing its catalytic activity in the microwave environment. Moreover, the order of reaction and activation energy were found as 0.33 and 44.9 kj*mol^{-1}, respectively. The synthesized catalysts were further characterized by XRD and SEM analysis.

Keywords: *Hydrogen, Microwave, Sodium Borohydride, Ni-B Catalyst*

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The Relationship Between Radon Gas Emanation and Earthquake on the Active Fault System

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Abstract: In this work, the possible relationship between radon anomalies and the earthquake on the active fault systems have been summarized. There are many published research articles showing that the radon activities are clearly high in some areas such as geological fault systems, geothermal sources, uranium deposit and volcano areas [1, 2]. Radon anomalies can be continuously detected with basic detection systems which are constructed especially on the fault system. The data were taken in each specified interval of time and then those time series were analyzed by using statistical methods. Some determined results were presented and the various-best used detection system over the world and some developed detection system for this purpose in Turkey were explained.

Keywords: *Radon emanation, earthquake, radon detection system.*

References:

[1] Al-Tamimi, M.H., Abumurad, K.M., Radiat. Meas. 34 (2001) 397–400.

[2] Inceöz, M, Baykara, O., Aksoy, E., Doğru, M., Radiat. Meas. 41 (2006) 349 – 353.

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Investigation of Ground-State Nuclear Structure Properties of Some Radionuclides Used in Nuclear Battery Technology

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Abstract: We investigated nuclear structure properties of radionuclides used in nuclear battery technology, such as binding energies per particle, the root mean square (rms) proton, neutron and charge density radii, and their density functions. Because, these radionuclides were used in spacecraft and space-probes as radioisotope thermoelectric generator, and in microelectronic technologies as betavoltaic batteries. In the calculations, we used Hartree-Fock approach for different force parameters, S3, T3, SKM*, SLY4, SLY5, SLY6 and SLY7. The calculated results were compared with the experimental data and theoretical relativistic mean field theory (RMFT). Based on the obtained results, we discussed force parameters and proposed new parameters [1].

Keywords: *Nuclear Battery, Nuclear Structure*

References:

[1] Artun, O., Modern Physics Letter A, Vol. 32, No. 22 (2017) 1750117.

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Investigation of Heavy Metal Concentrations in Soils at the Central Settlements of Erzincan- Turkey

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Abstract: Heavy metals are a natural component of the Earth's crust, but anthropogenic sources alter their geochemical structures such as industrial wastes, vehicle exhausts, municipal wastes, erosion of buildings and asphalt surfaces, dust deposits, suspended particles and coal burning activities. Heavy metal pollution in soil extremely affects crops quality, animals, human health, and eventually entire environment due to living beings interact directly with urban areas. In Erzincan, the dominant sources of heavy metal soil contamination are pesticide and fertilizer applications, animal feeds and manure, and mining. In this study, soils from Erzincan urban fields were chemically analyzed to determine concentrations of 8 heavy metals and further the intensity of pollution. For this purpose, soil samples were collected from 42 random points in the province of Erzincan center, district and villages. After the ground was cleared of stones, pebbles, vegetation and roots, 1 kg of specimen from the first 10 cm of topsoil was obtained within 40 cm2 each sampling site. Elemental analysis was conducted to determine As, Cd, Co, Cr, Cu, Ni, Pb and Zn concentrations using Wavelength Dispersive X-Ray Fluorescence (WDXRF) spectrometer (Axios Advanced 4, PANalytical, Netherlands). The obtained average concentrations of As, Cd, Co, Cr, Cu, Ni, Pb and Zn were 9.43±0.42, 6.1±5.12, 52.2±0.70, 739.6±14, 51.3±1.13, 638.4±12, 14.2±0.35 and 85.7±0.91 μg/g, respectively. The average values of the investigated elements are above average abundances of elements in the Earth's crust. High metal concentrations particularly are located in industrial and agricultural areas that indicate the major anthropogenic pollution sources are cement factories, fertilizers, mining processes, and traffic emissions.

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Keywords: *Anthropogenic pollutions, Erzincan, Heavy metals, Soils, XRF*

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Experimental and Quantum Chemical Studies of 2,2'-Bipyridyl-Linked Diamino Compound

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Abstract: The chemistry of diamino compounds containing 2,2'-bipyridyl unit in their framework is a fascinating area of research for the development of the Schiff-base ligands and metallosupramolecular chemistry [1,2]. The synthesis of the Schiff-base ligands recently have taken more attention in bioinorganic and bioorganic in medicine because of the fact that it has antimicrobial and chemotherapy features besides they are used in different industrial areas: Environment chemistry, agriculture, and paint industry.

In the present work, we report an experimental and theoretical approaches on versatile diamino compound containing 2,2'-bipyridine unit (Figure 1). The structure of diamino compound, 6,6'-bis(2-aminothiophenoxymethyl)-2,2'-bipyridine, was elucidated on the basis of elemental analysis, IR, 1H-NMR, 13C-NMR, and FAB mass spectra. Then, a complete description of the structural properties of the compound through its consistency with the spectroscopic data has been presented by quantum chemical methods. Structural and energetic properties of the compound have been investigated by Hartree-Fock and Density Functional Theory (B3LYP) with 3-21G and 6-311++G(d,p) basis sets [3]. Energies for the highest occupied molecular orbitals (HOMO), the lowest unoccupied molecular orbitals (LUMO) and HOMO-LUMO gaps have been obtained.

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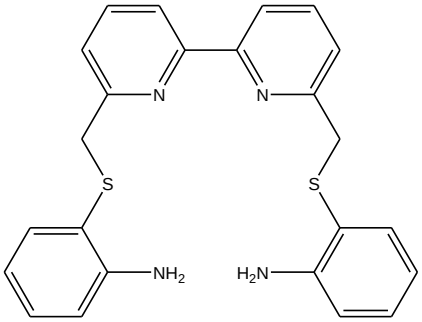

Figure 1. 6,6'-*Bis*(2-aminothiophenoxymethyl)-2,2'-bipyridine

Keywords: *2,2'-bipyridyl, HF, DFT.*

References:

[1] Rezaeivala, M. and Keypour, H. Coord. Chem. Rev., 280, 203–253, (2014).

[2] Glasson C.R.K., Lindoy L. F. and Meehan G. V., Coord. Chem. Rev., 252, 940–963, (2008).

[3] Frisch, M. J., *et. al*., Gaussian 03, Revision D.01 (Wallingford, CT: Gaussian Inc.) (2004).

Electronic Letters on Science & Engineering 13 (2) (2017)
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Dynamic Magnetic Hysteresis Behaviors in a Mixed Spin (3/2, 2) Bilayer System with Different Crystal-Field Interactions

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Abstract: We investigate the dynamic magnetic hysteresis loop behaviors of the mixed spin-3/2 and spin-2 Ising model with different crystal-field interactions under a time-varying magnetic field on a two-layer square lattice within the framework of dynamic mean-field calculations based on the Glauber–type stochastic dynamics. The dynamic magnetic hysteresis loops are obtained for different reduced temperatures (T), magnetic field amplitudes (h), frequencies (w) and interlayer coupling constants (J3). Influences of the T, h, w and J3 on the dynamic magnetic hysteresis loop properties are investigated. We also study the temperature, frequency and interlayer coupling interaction dependence of the coercive field and remanent magnetization. We compare our results with some theoretical and experimental works and observe a quantitatively good agreement with some theoretical and experimental results.

Acknowledgement. This work was supported by Erciyes University Research Fund, Grant No: FBA-2016-6324.

Keywords: *Mixed spin (3/2, 2) bilayer system, dynamic magnetic hysteresis, coercive field, remanent magnetization, Glauber-type stochastic dynamics, mean-field theory*

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Theoretical Calculation of Bulk Structure Properties for InSe/GaSe Semiconductor Heterostructures

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Abstract: In this study, the lattice constants and total energy calculations of β-InSe and β-GaSe systems in the hexagonal structure semiconductors were calculated using the plane wave of self-consistent field program based on the density functional theory. The lattice constants for these systems were found to be 7.309 au and 7.825 au, respectively. Also, the hexagonal structure c/a values were calculated to be 4.362 and 4.367, respectively. The calculations are based on intensive computer use and simulation calculations. Using the information obtained from these calculations, an InSe/GaSe bulk heterostructure was formed in the z direction. The lattice constant of this system was found to be 7.528 au and c/a value of 8.769 as a result of the optimization calculations made.

In addition, the first and second averages of the electrostatic potential curves of this system have calculated and the difference between these potential curves has found to be $\Delta V = 0.365$ Ry. Due of this potential difference, heterostructures are suitable for forming quantum wells at low dimensions. Thus, these systems are thought to be used in the construction of opto-electronic and nano-electronic devices.

Keywords: *β-InSe, β-GaSe and InSe/GaSe Semiconductors, Bulk Properties, Density Functional Theory*

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Theoretical Investigation on the NbRuB and NbOsB Compounds

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[2]*Aksaray University, BOTE, TR68100, Aksaray, Turkey*

Abstract: We report a comprehensive theoretical study on the mechanical and phonon properties of orthorhombic NbRuB and NbOsB compounds within the framework of density functional theory. Generalized gradient approximation has been used for modelling exchange-correlation effects. The elastic constants, bulk modulus, shear modulus, Young's modulus, Poisson's ratio, Debye temperature, shear anisotropic factors and the elastic anisotropy are obtained and analyzed for the first time. Furthermore, the phonon spectra, phonon density of states, and thermal conductivities are also discussed. Our results are in agreement with the available experimental and theoretical data.

Acknowledgements. This work is supported by Aksaray University, Scientific Research Project Commission, through grants 2016-037.

Keywords: *ab initio, NbRuB, NbOsB*

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Theoretical Reaction Mechanism Study of 5-Methoxyisatin-3-(N-Phenyl)Thiosemicarbazone Derivatives and 2,2-Diphenyl-1-Picrylhydrazyl Radical

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Abstract: In this study, a theoretical investigation was performed to understand the reaction mechanism between the 5-Methoxyisatin-3-(N-phenyl)thiosemicarbazone (H2MIPT) and 5-Methoxyisatin-3-(N-chlorophenyl)thiosemicarbazone (H_2MICPT) with 2,2-Diphenyl-1-Picrylhydrazyl (DPPH) radical in the gas phase using molecule based reaction approach with PM6 method by using Gaussian 09W [1] software package. H2MIPT-DPPH reactants go to an H2MIPTDPPH molecule via a transition state structure TS. The energy profiles of the reactions H_2MIPT-DPPH → H2MIPTDPPH and H2MICPT-DPPH are given in Figure 2. In both cases, only one transition state (TS) proceeded by a shallow minimum of the prereaction complex (TS), occurs between the addends and the product minima.

This involves an increase in energy by 0.022278 au for path TS (H2MIPTDPPH) and by 0.021953 au for path H2MICPT DPPH. Stationary points were checked by vibrational frequency analyses to see whether they constituted minima or maxima on the PES. Both transition structures showed a single imaginary frequency (Imaginary frequency of TS for H_2MIPTDPPH and H_2MICPT DPPH is -138 cm^{-1} and -101 cm^{-1}.

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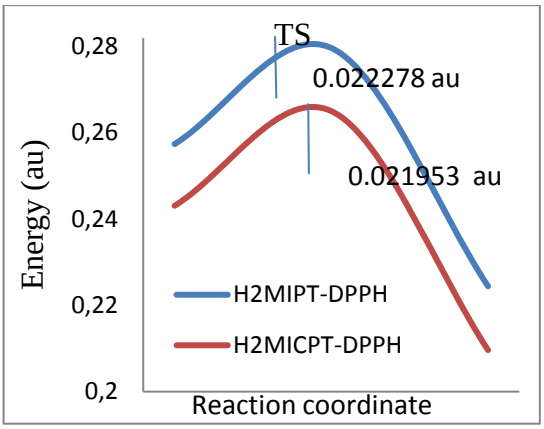

Figure 1. Reaction coordinate

Keywords: *Isatin, thiosemicarbazone, DPPH*

References:

[1] M. J. Frisch, *et. al*., Gaussian 09, Revision A.1, Gaussian, Inc., Wallingford CT, 2009.

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Theoretical Study of Corrosion Inhibition for Benzaldehyde Thiosemicarbazide, p-Chlorobenzaldehyde Thiosemicarbazide and 4-Dimethylaminobenzaldehyde Thiosemicarbazide

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[2]*Biomedical Engineering Department, Faculty of Engineering and Architecture, Kastamonu University, TR37150 Kastamonu, Turkey*

Abstract: The recent use of theoretical chemistry to explain the mechanism of corrosion inhibition, such as quantum chemistry calculations has proved to be a very powerful tool for studying the mechanism of different systems. In this study, quantum chemical parameters such as the highest occupied molecular orbital energy (E_{HOMO}), the lowest unoccupied molecular orbital energy (E_{LUMO}), the energy gap between E_{LUMO} and E_{HOMO} (ΔE), chemical hardness, softness, electronegativity, electrophilicity, chemical potential, nucleofugality, electrofugality and polarization for benzaldehyde thiosemicarbazide p-chlorobenzaldehyde thiosemicarbazide, 4-dimethylaminobenzaldehyde thiosemicarbazide, were calculated based on DFT method. For this approach one has used several different functionals and basis set such as RHF-B3LYP / 6-311g (d, p) and rhf-B3LYP / 6-311 ++ g (2d, 2p) on rb-B3LYP / 6-311 ++ g (2d, 2p) and rb-B3LYP / 6-311g (d, p). The data obtained from quantum chemical calculations and experimental efficiencies of inhibitors [1] were subjected to evaluate a correlation analysis. Among other properties Table (1) summarizes our preliminary results:

Tablo 1: Correlation between experimental and theoretical inhibition value

Compounds	E_{HOMO} (R^2)	E_{LUMO} (R^2)	Polarizability (R^2)
natural	0.9995	0.9992	0.9992
pronated	0.9996	0.9995	0.9993
Natural water	0.9998	0.999	0.9990
pronated water	0.9998	0.9995	0.9989

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Keywords: *Corrosion, therotical study, organic inhibitors*

References:

[1] Abd-El-Nabey, B. A., et. al., Int. J. Electrochem. Sci., 7 (2012) 11718-11733.

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QSAR Study on Thiosemicarbazone Derivatives as Ribonucleotide Reductase Inhibitors

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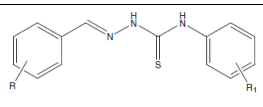
Abstract: QSAR analysis on thiosemicarbazone derivatives exposing RNR inhibitory activities [1] were performed. In this series of 21 compounds, 13 of them were reported with inhibitory concentration (IC50) in the l M range. The inhibitory concentration of those compounds were converted into -logIC50 before being correlated with the structural features.

The quantum chemical calculations have been carried out at the B3LYP level of theory using Gaussian-09 series of program package. The density functional theory (DFT), with the Becke's three parameter exchange functional along with the Lee– Yang–Parr correlation functional (B3LYP) were performed in order to calculate the quantum chemical descriptors such as HOMO, LUMO, Energy gap, Hardness, Softness, Chemical potential and Dipole moment of the investigated molecules. Calculated descriptors for some thiosemicarbazone derivatives were given in Table 1.

Tablo 1: Some descriptor calculations of thiosemicarbazone derivatives

		HOMO	LUMO	Energy gap	Hardness	Softness	chemical potential	Dipole moment
2-OH	H	-0.218	-0.079	0.139	0.070	14.380	0.063	6.536
2-OH	4-Cl	-0.260	-0.083	0.177	0.088	11.305	0.092	7.953
4-OH	H	-0.217	-0.074	0.143	0.071	14.020	0.075	6.122
4-OH	4-Cl	-0.221	-0.078	0.143	0.072	13.983	0.066	7.725
3-OCH3-4-OH	H	-0.250	-0.072	0.178	0.089	11.265	0.089	6.171
3-OCH3-4-OH	4-Cl	-0.217	-0.076	0.140	0.070	14.244	0.073	8.088
2-Furyl	H	-0.220	-0.080	0.140	0.070	14.264	0.071	6.171

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Keywords: *QSAR, Thiosemicarbazone, RNR inhibitory*

References:

[1] Moorthy N. S. H. N., Cerqueira N. M. F. S. A., Ramos M. J., Fernandes P. A., Med. Chem. Res. 21 (2012) 739–746.

Electronic Letters on Science & Engineering 13 (2) (2017)
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The Morphologics Properties of as-Cast and Melt-Spun Al-5Zn-2.5Mg Alloy

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Abstract: The rapid solidification processing (RSP) involves exceptionally high rates of cooling (10^4–10^8 K/s) during solidification from the molten state. The RSP allows a reduction in grain size, extended solid solution ranges, reduced levels of segregation and, in some cases, the formation of metastable crystalline and amorphous phases. The levels of undercooling achievable at such high cooling rates lead to significant and often potentially beneficial modifications to rapidly solidified microstructures compared with those produced under conventional conditions. On the other hand, the rapidly solidified Al-Zn-Mg materials have attracted considerable attention owing to their excellent physical, chemical, mechanical and tribological properties, such as high hardness, enhanced elastic modulus, very low friction coefficient, low surface energy, supercorrosion and wear resistance, and low electrical and thermal conductivity. In this study, the microstructure of conventionally and rapidly solidified Al-5Zn-2.5Mg alloy was investigated. The microstructures of the Al-5Zn-2.5Mg alloy were characterized by the SEM and the phase composition was identified by the XRD analysis. The phase transition during the solidification process was studied by the DTA under an Ar atmosphere. The XRD patterns for the conventional solidified (CS) Al-5Zn-2.5Mg sample revealed three phases, the two intermetallic phases ($Al_{12}Mg$ and $MgZn_2$) and the α –Al phase. While no peaks corresponding to intermetallic phases for the MS ribbons obtained with wheel speed of 80m/s. The SEM analysis showed that the CS sample has dendritic α-Al solid solution and non-equilibrium phases. On the other hand, the MS ribbons of 80 m/s wheel speed showed more homogeneity than that in CS sample. The melting temperature for MS ribbons with the wheel speed of 10 and 80 m/s were 660 ºC and 662 ºC, respectively. Finally, it has been found that the ribbon thickness has an inverse proportional to the melt spun wheel speeds.

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Keywords: *Al-5Zn-2.5Mg alloy, Rapid solidification, Microstructure*

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Fabrication and Characterizations of Dysprosium-Doped Cubic Zirconia Films via Slurry Spin Coating for IT-SOFC

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Abstract: In the present study, it was aimed that the production, characterization, optimization and improving the thick film properties of Dy_2O_3 doping ZrO_2-based solid electrolyte system. In this way, $(ZrO_2)_{1-x}(Dy_2O_3)_x$ ($0.02 \leq x \leq 0.12$) binary system have been synthesized with a Pechini method as the electrolyte material to use in solid oxide fuel cells (SOFCs). The cubic phase of the $(ZrO_2)_{1-x}(Dy_2O_3)_x$ ceramics was obtained as 8-12 mol% of dysprosium ions. Thick films of the *fcc*-ZrO_2 type powders were produced by using of the ethyl cellulose organic binder mixture and the spin coating method. The produced DySZ thick films were characterized with the thickness and the homogeneity which are depending on the nature of the DySZ slurry (viscosity, surface tension, volatility of solvent system, solid loading, slurry homogeneity, etc.) and the spin coating parameters (spin rate, rotation period, etc.). The properties of the DySZ slurry were fixed for all the samples. All of the coating parameters were optimized and determinated with pre-coating treatments. The calcination and the crystallization behaviour was studied by X-ray diffraction (XRD). The thermal decomposition of the films was investigated by TG/DTA analysis. The grain sizes and the thicknesses of the films were estimated by scanning electron microscopy (SEM).

Keywords: *ZrO_2, Dy_2O_3, Pechini method, Spin coating, Solid oxide fuel cell (SOFC)*

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Electron Dynamics in Metal Nanoclusters Under Optical Vortices

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Abstract: The intention of this work is to observe the effect of the spatial profile and angular orbital momentum characteristics of the optical vortex on quantum sized, spherically symmetric metal clusters. Particularly, surface states localized near the surface and image-state electrons which are originated in the long range nature of the image potential outside a solid in metal nanoclusters can be strongly manipulated by transferring orbital angular momentum [1] of optical vortex. The possibility of transfer of angular momentum of light into the molecular structures has been studied in our previous works [2-4].

In this study, the electronic structure of a monovalent atomic system was calculated. The model potential known as Chulkov potential was used as confinement potential [5]. In order to obtain electronic structure and radial eigenfunctions of metal nanoclusters shooting method was performed. The interaction between light and cluster has been calculated by time dependent perturbation theory. Light induced change in electron dynamics is strongly related to light frequency, spin and orbital angular momentum of light.

Keywords: *Optical vortex, metal nanoclusters, electron dynamics, surface and image states*

References:

[1] K. Köksal, and J. Berakdar, Phys. Rev. A 86, 063812 (2012).

[2] K. Köksal, and F. Koç, Phil. Mag. 96, 2686 (2016).

[3] K. Köksal, and F. Koç, Comp. and Theor. Chem. 1105, 27 (2017).

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[4] K. Köksal, and F. Koç, Comp. and Theor. Chem. 1099, 203 (2017).

[5] E.V. Chulkov, V. M. Silkin, and P. M. Echenique, Surface science 437, 330 (1999).

Electronic Letters on Science & Engineering 13 (2) (2017)
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A Molecular Dynamics Study about the Physical Properties of Co_mAu_n (m+n=147) Nanoclusters with the Icosahedral Shape

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Abstract: In recent years the usage of metallic nanoparticles in biomedicine is an attractive research area [1, 2]. Binary metallic particles, especially core-shell configuration with a magnetic core (i.e., Co, Ni, and Fe) and a biocompatible shell (i.e., Au) can present a more robust structure for novel biomedical applications [3,4]. The thermodynamic stability of nanoparticles to be used in biological applications needs to be examined very well. We used classical molecular dynamics simulations in canonical ensemble conditions (NVT) keeping the temperature constant with Andersen thermostat for investigation of dynamical properties of bimetallic Co-Au nanoalloy clusters with the interatomic interactions modeled by Gupta many-body potential. It requires to obtain the atomic configuration with the lowest potential energy of cluster corresponding to the Global Minimum on the potential energy surface. Global optimizations were performed using basin-hopping algorithm for Co_mAu_n, m+n=147 bimetallic clusters. Structures based on icosahedron were obtained for all compositions. The icosahedral structures were taken as the initial configurations for MD simulations which gives the structural evolution of the Co-Au nanoclusters during the heating process is investigated in detail. We obtained caloric curves (cluster potential energy versus temperature) and Lindemann parameters (The Lindemann index, i.e., the root-mean-square bond-length fluctuation) to determine the melting temperatures. We have compared the melting-like transitions of Co-Au nanoalloys for all compositions. The common neighbour analysis of configurations obtained by MD simulations shows that the solid to solid transitions occur in some compositions of Co-Au nanoalloys before melting transitions. Co-Au binary metal nanoalloys mostly prefer Co core and Au shell segregation. The excess energy analysis indicates that $Co_{55}Au_{92}$ is the most stable composition.

Keywords: *nanoalloy, optimization, melting.*

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References:

[1] B.D. Chithrani, A.A. Ghazani, W.C.W. Chan, Nano Lett. 6 (2006) 662.

[2] W.S. Seo, *et. al*., Nat. Mater. 5 (2006) 971.

[3] S. Kayal, R.V. Ramanujan, J. Nanosci. Nanotechnol. 10 (2010) 5527.

[4] J.-I. Park, J. Cheon, J. Am. Chem. Soc. 123 (2001) 5743.

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Hydrogen Generation by Hydrolysis of Sodium Borohydride

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Abstract: Generation of hydrogen from hydrolysis of borohydrides is important. Many works are appearing about this topic. Uses of catalysts have great effect on hydrogen generation ratio. We studied effect of micro sized Ir(0) catalyst on rate and amount of generated hydrogen. We also, studied the effect of stirring and hydroxide concentration on rate and yield. An experimental set up apparatus was obtained for measurement of released hydrogen. Spectroscopic methods applied for characterization of catalyst [1]. Effect of each parameter on generation of hydrogen was outlined and optimum reaction conditions were obtained.

Keywords: *Hydrogen generation, Ir(0) catalyst*

References:

[1] Aksu M., Asian Journal of Chemistry; Vol. 26, No. 23 (2014) 8181-8184.

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Synthesis, Characterization and Quantum Chemical Calculations of 4-Tert-Butylphenol-Methylboronic Acid and Antioxidant Applicatıons

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Abstract: The boron and boronic acids are still an increasing interest due to their extensive and important applications in various interdisciplinary area. A wide range of biologically importance of boronic acid derivatives have been synthesized as anti-metabolites. The boronic acid moiety was also incorporated into amino acids and nucleosides as anti-tumor, anti-viral agents [1-2]. In this study, 4-tert-butylphenol-methylboronic acid have been synthesized. The resulting compounds were characterized by different methods (Figure 1). Antioxidant properties of this synthesized compound was analyzed. Moreover, structural and energetic properties of the conformers of compound (Figure 2) have been investigated by Hartree-Fock and Density Functional Theory (B3LYP and PBE) with 6-311++G(d,p) basis set [3]. Energies for the highest occupied molecular orbitals (HOMO), the lowest unoccupied molecular orbitals (LUMO) and HOMO-LUMO gaps have been computed. It was found that experimental and calculated IR values are in good agreement.

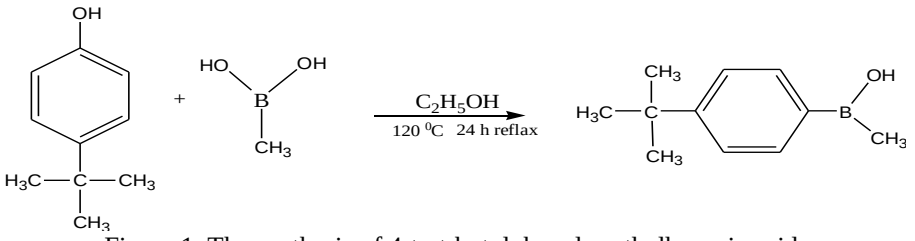

Figure 1. The synthesis of 4-tert-butylphenol-methylboronic acid.

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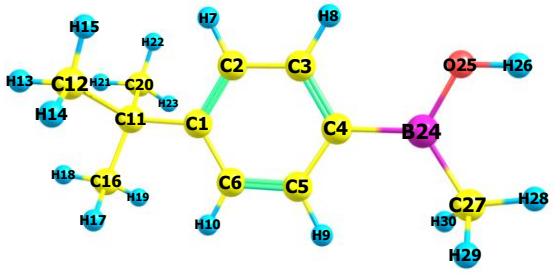

Figure 2. Optimized geometry of 4-tert-butylphenol-methylboronic acid.

Keywords: *4-tert-butylphenol, methyl boronic acid, HF, DFT.*

References:

[1] W. Tjarks, *et. al*., J. Med. Chem., 35 (1992) 16228.

[2] X. Chen, *et. al*., J. Phys. Org. Chem., 11 (1998) 378–386.

[3] M. J. Frisch, *et. al*., Gaussian 03, Revision D.01 (Wallingford, CT: Gaussian Inc.) (2004).

Electronic Letters on Science & Engineering 13 (2) (2017)
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Antioxidant and Morphological Characteristics of ZnO Nanoparticles Using Tangerine Extract

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Abstract: The synthesis of metal and semiconductor nanoparticles is an expanding research area due to the potential applications in the development of novel technologies. Especially, green synthesized nanomaterial has become an important branch of nanotechnology. Several chemical and physical techniques have been utilized for the synthesis of metallic nanoparticles, which have some negative effects causing to toxicity in the environment. These methods have the unhealthy aspect of using chemical or organic complexes as the reducing agents, which can be harmful to the environment. Plants extracts provide a green synthesis procedure of ZnO nanoparticles, which are more eco-friendly, harmless to the environment and allows a controlled synthesis with well-defined size and shape of nanoparticles. The present work, described the synthesis of zincoxide nanoparticles (ZnO NPs) using shell aqueous extract of tangerine and its antioxidant activities. The nanoparticles were obtained characterized by UV–Vis spectroscopy, X-ray diffraction (XRD), Energy dispersive X-ray analysis (EDAX) and Field emission scanning electron microscopy (FESEM) analysis. In this study we also investigated antioxidant of green synthesized ZnO NPs. The XRD patterns illustrated a single phase hexagonal (wurtzite) structure. The FE-SEM micrographs revealed the formation of erythrocyte-like structures and the average particle sizes were found to be 50–150 nm. The UV-vis measurements showed that the average optical transparency is over 80% in the visible range. ZnO nanoparticles were showing antioxidant properties.

Keywords: *ZnO NPs, Green synthesized, Antioxidant*

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Investigation of the Effect on the Relaxation Times of Albumin Aggregation in D_2O Solutions

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Abstract: This study was carried out to explain the effect of albumin aggregation to T1 and T2 relaxation times and mechanisms leading to relaxation. Existence of albumin aggregation was investigated in terms of Inversion Recovery (IR)-T1 FID signals, Spin Echo (SE)-T_2 signals and decay curves. In the experiment, Human serum albumin and Deuterium Oxide (D_2O) solvent which includes 0,1 % residual water, were used. Concentration measurements were made in two groups by adding different amount of albumin to 1 ml of D_2O. Concentrations; In the first group, albumin was added as 0.02 g up to 0.1 g, while in the second group, it was changed from 0.1 g to 0.5 g. Measurements were made with Bruker Avance 400 MHz 1H-NMR spectrometry. T1 measurements were conducted by IR method, whereas T_2 measurements were carried out by CPMG method.

FID and SE qatars of D_2O exhibit a single exponential change, which has seen from FID, Echo sets and IR-T_1, SE-T_2 curves. However, when the amount of album was increased, exponential appearance of FID and SE qatars changed. It showed that protein aggregation increases at high concentrations. Concentrations of up to 10 % of the samples of IR-FID, SE-T_1 qatars and IR-T_1, SE-T_2 curves perfectly fit with related formulas. This situation revealed that T_1, T_2 experiments can be performed by using albumin up to % 10 concentrations. Signal decays after 20 % concentration on the IR-T_1 and SE-T_2 curves became apparent, which showed that protein aggregation is very effective at 20 % and higher concentrations.

Keywords: *T1, T2, NMR, Albumin aggregation, Inversion Recovery*

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High Energy Accelerator Studies in Turkey

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Abstract: We explain recent simulation studies and technical improvements on high energy accelerator technology in the research centers of universities and technology companies in Turkey. Vacuum studies and technologies, magnet systems with including dipole, quadrupole, solenoid, and undulator etc., superconducting and normal conducting cavity cells design, water cooling systems, control systems, radiation safety studies, clean room requirements, dump systems, diagnostic system both for beam and radiation, various experimental room designs and experiments, all of them are explained and summarized in more detail in this research. Especially, vacuum system requirements are well known and system parts for high energy accelerators can be produced and diagnose in Turkey while some other country helps are needed for superconducting and normal conducting cavity cell manifacturing. Also undulator magnet production and alignments can be made in Europe. We study and make simulations of whole accelerator system starting from photocathode gun to laser production and we will present our simulation studies in this workshop.

Keywords: *High energy accelerators, superconducting cavity, vacuum system, radiation safety, dump system*

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A DFT Study of Hexagonal Mg^{+2} Doped Fluorapatite $Mg_xCa_{10-x}(PO_4)F_2$ ($0 \leq x \leq 4$)

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Abstract: Mg^{+2} doped fluorapatite has great importance to the development of biomaterials in which chemical composition is as close as possible to that of bone [1]. The application of geometry optimization of hexagonal Mg^{+2} doped $Ca_{10}(PO_4)F_2$ fluorapatite (FAP) has been investigated by using density functional theory (DFT) method in this study. All calculations were performed using the Perdew-Burke-Ernzerhof (PBE) functional and STO-3G basis sets [2]. First, the lattice parameters and equilibrium volumes for FAP have been calculated with a hexagonal structure. The Mg^{2+} ions have been partially substituted Ca^{2+} in the FAP's unit cells. The full range of Mg^{+2} doped fluorapatite from $Ca_{10}(PO_4)_6F_2$ to $Mg_4Ca_6(PO_4)_6F_2$ have been studied with the selected methodology. The calculations have been carried out to determine the lattice constants, vector angles, the chemical bond lengths and O-P-O bond angles for each composition. Moreover, O_3-Ca_2-F bond angles have been computed for pure FAP. It has been observed that the lattice constant value decreases and the bond lengths increase with the increasing number of Mg^{+2} ions for $Mg_xCa_{10-x}(PO_4)F_2$ ($1 \leq x \leq 4$). The lattice constants and the bond lengths computed here are approximately in the range of 0.1–0.2 Å and 0–0.1 Å, respectively, which are larger than the theoretical and experimental data reported in literature for pure FAP [3, 4]. On the other hand, the determined vector angles are almost the same with the experimental data for pure FAP [3].

Keywords: *FAP, DFT, $Mg_xCa_{10-x}(PO_4)F_2$*

References:

[1] S. Nasr and K. Bouzouita, Bioinorganic Chemistry and Applications, 2011 (2011) 453759.

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[2] M. J. Frisch, *et. al*., Gaussian 03, Revision D.01 (Wallingford, CT: Gaussian Inc.) (2004).

[3] J. M. Hughes, M. Cameron, K.D. Crowley, American Mineralogist, 74 (1989) 870.

[4] H. Njema, *et. al*., Materials Research Bulletin, 51 (2014) 210.

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Multi-Focus Image Fusion Based on Discrete Wavelet Transform Using Firefly Optimization Algorithm

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Abstract: Multi focus image fusion (MFIF) is to obtain an image with more information and sharpness from multi focus images (MFI). This paper proposes a image fusion method for MFIF based on discrete wavelet transform (DWT2) using firefly optimization algorithm (FOA). Wavelet transform is a mathematical tool developed originally in the field of signal processing and is used widely in image processing. Proposed method consists of three parts. First step of all, DWT2 is applied to the all multi focus images separately. Next, the fusion rate of DWT2 applied images are optimized using FOA. FOA has been created by inspiring social behaviours of firefly to solve nonlinear global optimization problems. For the FOA's evaluation function, is selected a function which is maximized variance values of fusion image and minimized the sum-modified laplacian value of fused image. Then, the fusion rate of multi focus images is optimized using FOA. At the last step, fused image is obtained from applying inverse DWT2 to DWT2 images according to the optimized fusion rate. The proposed method was used first time in the literature for MFIF based on DWT2 using FOA. The proposed method is applied to the multi focus images obtained from the literature and shows that more effective results than conventional methods such as selecting the maximum values from DWT2 images and selecting the average values from DWT2 images and results are shown in Fig 1.

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Keywords: *Multi Focus Image Fusion (MFIF), Discrete Wavelet Transform (DWT2), Firefly Optimization Algorithm (FOA).*